Stress analysis of elastically anisotropic bilayer structures

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In this paper, a newly developed model for analyzing stresses and curvatures in elastically anisotropic bilayer structures is presented. This model can be applied to bilayer structures composed of a single thin film that is deposited or grows on an elastically anisotropic substrate. The thin-film materials considered can be either elastically isotropic or anisotropic. According to this model, the Young's modulus, Poisson's ratio, and thermal-expansion coefficient of any given thin film cannot be determined independently by simply using a single elastically anisotropic substrate in a stress measurement without making additional assumptions. By using our model and with reasonable assumptions, more reasonable values of the mechanical constants and thermal-expansion coefficient of the aluminum thin film have been recalculated from the results of Janda [Thin Solid Films **112**, 219 (1984)].

I. INTRODUCTION

Thin-film materials have been widely used in many applications.[1–6] They can be metals, semiconductors, polymers, or ceramics. Though most of their properties, especially mechanical properties, are well known in bulk, much more needs to be studied about these properties in thin films. The mechanical properties as well as the residual stresses in thin films may significantly vary with different processes, processing conditions, and thermal histories. Therefore, it is important to investigate these mechanical and stress characteristics in thin films experimentally. In the meanwhile, correct formulas or theoretical models must be applied.

For the above-mentioned purposes, many experimental and theoretical works have been done.[7–24] Among these, stresses in thin-film materials have been studied most extensively.[7–12] As can be seen, all those thin films were prepared on elastically isotropic substrates for a few practical reasons. However, in order to obtain the biaxial moduli and thermal-expansion coefficients of the films *in situ*, two different substrates have been used.[7,8] Otherwise, assumptions must be made so that either biaxial modulus or thermal-expansion coefficients of the thin film and substrate can be estimated, if a single elastically isotropic substrate is used.[9–12] This can be done, for example, by assuming that the thermal-expansion coefficients of the thin films are the same as those of the bulk. If this is true, the corresponding biaxial moduli can then be calculated.[9,10] As to measuring these properties *in situ* on the substrate, these are the only two approaches up to now, though there are some other alternatives.[13–15]

In his paper,[16] Janda has tried a different approach to measure these properties *in situ*, that is, by using a single elastically anisotropic substrate. It is thought that both the biaxial modulus and thermal-expansion coefficient of any given thin film could be obtained simultaneously by using such an approach with no assumptions made elsewhere. If this were true, this approach might be a relatively convenient one. Unfortunately, the theoretical model presented for the approach is incorrect. After developing a new theoretical model for the same structure, we have noted that the approach does not have the expected feature just mentioned above. Furthermore, the biaxial modulus and thermal-expansion coefficient that Janda has calculated for the aluminum thin film are also incorrect.

Therefore, in this paper it will be discussed in detail how our model is established. As will be shown later, the biaxial modulus and thermal-expansion coefficient cannot be obtained simultaneously even using such an approach, according to our model. Assumptions must be made in order to determine the properties. It seems that this approach is not much different or better when compared with the other two methods mentioned earlier, though this approach still has its own uniqueness. Instead of the biaxial modulus, separated values of the Young's modulus and Poisson's ratio can be obtained, if the thermal-expansion coefficient of the given thin film is known or assumed to be equal to that of the bulk. The resulting Poisson's ratio can be used to back-verify the assumption made. On the other hand, if Poisson's ratio is known or assumed to be equal to that of the bulk, Young's modulus and the thermal-expansion coefficient can be individually determined.

II. THEORY

Several theoretical models[18–20] regarding stress analysis of a single layer of thin film deposited on an elastically isotropic substrate have been established since 1909. Appropriate stress models for multiple layers of thin films or multilayered structures were introduced in the 1980s.[21–24] All these models, though, consider only elastically isotropic structures. Nevertheless, from these models, a rule of thumb can be extracted for establishing an appropriate stress model for any given layered structure, no matter whether it is composed of single or multiple thin films, and whether its substrate is elastically isotropic or anisotropic. To develop a stress model like this, one can start with solving the equations of the balances of the internal forces, interfacial strains, and moments in the structure. The only difference between

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the isotropic and anisotropic cases is that in the latter case, three balance equations must be individually established in the two orthogonal directions in the plane (Fig. 1).

A. Internal force balance

If a thin film is deposited or grown on an anisotropic substrate, the internal force balances in the plane directions, x and y, can be expressed as

$$F_{1x} = -F_{2x}, \tag{1a}$$

$$F_{1y} = -F_{2y}, \tag{1b}$$

where the subscript "1" denotes the thin film and "2" the substrate.

B. Interfacial strain balance

From the balance of the strains at the interface of the thin film and the substrate, one has

$$X - \int_{T_i}^{T_f} \alpha_{2x} dT + \frac{F_{2x}}{WE_{2x}d_2} - \frac{\nu_{2y}F_{2y}}{WE_{2y}d_2} + \frac{d_2}{2R_x} = \int_{T_i}^{T_f} \alpha_{1x} dT + \frac{F_{1x}}{WE_{1x}d_1} - \frac{\nu_{1y}F_{1y}}{WE_{1y}d_1} - \frac{d_1}{2R_x}, \tag{2a}$$

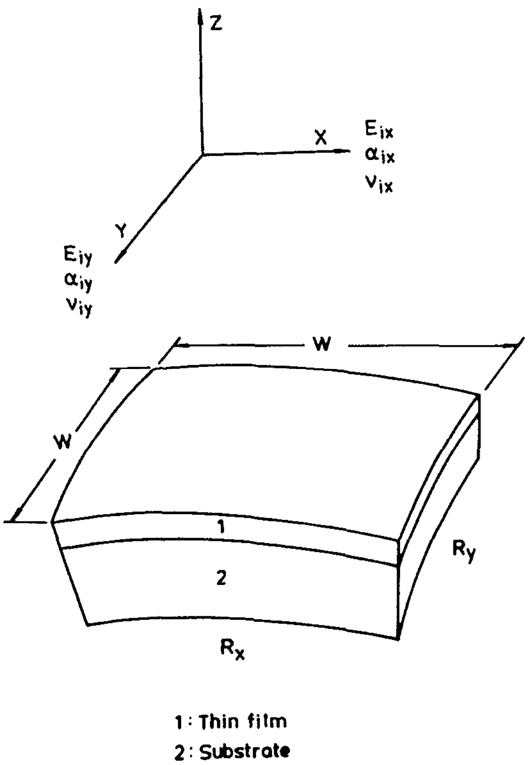

FIG. 1. Schematic illustration of a bilayer structure with a thin film deposited onto an elastically anisotropic substrate in the Cartesion coordinate system.

$$Y - \int_{T_i}^{T_f} \alpha_{2y} dT + \frac{F_{2y}}{WE_{2y}d_2} - \frac{\nu_{2x}F_{2x}}{WE_{2x}d_2} + \frac{d_2}{2R_y} = \int_{T_i}^{T_f} \alpha_{1y} dT + \frac{F_{1y}}{WE_{1y}d_1} - \frac{\nu_{1x}F_{1x}}{WE_{1x}d_1} - \frac{d_1}{2R_y}, \tag{2b}$$

where α denotes the thermal expansion coefficient, T_i and T_f are the initial temperature and the temperature at observation, respectively, E_1 is the tensile modulus of the thin film, E_2 is the Young's modulus of the substrate, ν is Poisson's ratio, d is the thickness, and W width. R is the radius of curvature of the structure and has a positive sign if bending downward, as shown in Fig. 1.

The first term on either side of Eq. (2) is to account for thermal strain due to thermal-expansion mismatch. If there exists intrinsic stress in the deposited film, an intrinsic strain term can be also added directly and the entire derivation will not be affected. If a deposited polymer film swells or expands upon taking up moisture or solvent, a hygroscopic strain term should be taken into account, similarly.

Upon cooling or heating, these forces will change according to the magnitude of the thermal mismatch between these two layers. These are the principal forces that keep the dimensions of the two layers matched in the plane direction. Since a two-dimensional structure is concerned, the forces in the y direction will affect the strain in the x direction. Due to elastic anisotropy, the forces in the x and y directions may not be the same. Such an anisotropic biaxial effect is expressed in the second force term in the above equation. The last terms on both sides of the equation account for strain variations due to bending.

From Eqs. (1) and (2), the internal forces can be obtained readily and expressed as functions of the thermal mismatch and radii of curvature in both x and y directions:

$$F_{1x} = \frac{C_x B_y - C_y B_x}{A_x B_y - A_y B_x}, \tag{3a}$$

$$F_{1y} = \frac{A_x C_y - A_y C_x}{A_x B_y - A_y B_x}, \tag{3b}$$

where

$$A_x = (1/E_{1x}d_1 + 1/E_{2x}d_2),$$
$$A_y = -(\nu_{1x}/E_{1x}d_1 + \nu_{2x}/E_{2x}d_2),$$
$$B_x = -(\nu_{1y}/E_{1y}d_1 + \nu_{2y}/E_{2y}d_2),$$
$$B_y = (1/E_{1y}d_1 + 1/E_{2y}d_2),$$
$$C_x = W\left(\int_{T_i}^{T_f} (\alpha_{2x} - \alpha_{1x}) dT + \frac{d_1 + d_2}{2R_x}\right),$$
$$C_y = W\left(\int_{T_i}^{T_f} (\alpha_{2y} - \alpha_{1y}) dT + \frac{d_1 + d_2}{2R_y}\right).$$

C. Moment balance

In such a bending structure, there are two different kinds of moments. The first kind originates from the internal forces, and is balanced by the bending moments of the structure. From the balance of the moments, one has

$$M_{1x} + M_{2x} + F_{1x}(d_1/2) + F_{2x}(d_1 + d_2/2) = 0, \tag{4}$$

where M denotes the moment due to bending. For an isotropic structure, its bending moment has long been understood and can be obtained readily. For an anisotropic structure, some manipulations are needed. The bending moments can be obtained according to the following relations. First, the bending moment and the stress due to bending can be correlated as

$$M_{ix} = W\int_{-d_i/2}^{d_i/2} \sigma_{ixb} z\, dz, \tag{5}$$

where $i = 1,2$; $\sigma_{ixb} = K_{ixb}z$, and K_{ixb} is a constant.
At $z = d_i/2$,

$$\sigma_{ixb} = \sigma_{ixb}^{\max} = (6/Wd_i^2)M_{ix}, \tag{6}$$

where σ_{ixb} is denoted as the stress due to bending in the x direction. The expression correlating the bending moment and the bending stress in the y direction is similar and omitted here.

The next step is to correlate the bending stresses with the bending curvatures. The radius of curvature R_x and the maximum bending strain ϵ_{ixb} can be written, as usual, as

$$\frac{1}{R_x} = \frac{\epsilon_{1xb}^{\max}}{d_1/2} = \frac{\epsilon_{2xb}^{\max}}{d_2/2}. \tag{7}$$

According to Hooke's law, the maximum bending strains can be expressed as

$$\begin{aligned} \epsilon_{ixb}^{\max} &= \frac{\sigma_{ixb}^{\max}}{E_{ix}} - \frac{\nu_{iy}\sigma_{iyb}^{\max}}{E_{iy}} = \frac{d_i/2}{R_x}, \\ \epsilon_{iyb}^{\max} &= \frac{\sigma_{iyb}^{\max}}{E_{iy}} - \frac{\nu_{ix}\sigma_{ixb}^{\max}}{E_{ix}} = \frac{d_i/2}{R_y}. \end{aligned} \tag{8}$$

By combining Eqs. (6), (7), and (8), and after rearrangements, the bending moments can be related to the bending curvatures:

$$\begin{aligned} \frac{M_{ix}}{E_{ix}} - \frac{\nu_{iy}M_{iy}}{E_{iy}} &= \frac{Wd_i^3}{12R_x}, \\ \frac{M_{iy}}{E_{iy}} - \frac{\nu_{ix}M_{ix}}{E_{ix}} &= \frac{Wd_i^3}{12R_y}. \end{aligned} \tag{9}$$

From the above equation, the bending moments can be solved as

$$\begin{aligned} M_{1x} &= \frac{WE_{1x}d_1^3(R_y + R_x\nu_{1y})}{12R_xR_y(1-\nu_{1x}\nu_{1y})}, \\ M_{1y} &= \frac{WE_{1y}d_1^3(R_x + R_y\nu_{1x})}{12R_xR_y(1-\nu_{1x}\nu_{1y})}, \\ M_{2x} &= \frac{WE_{2x}d_2^3(R_y + R_x\nu_{2y})}{12R_xR_y(1-\nu_{2x}\nu_{2y})}, \\ M_{2y} &= \frac{WE_{2y}d_2^3(R_x + R_y\nu_{2x})}{12R_xR_y(1-\nu_{2x}\nu_{2y})}. \end{aligned} \tag{10}$$

From Eqs. (3), (4), and (10), and by assuming that $d_1 \ll d_2$ and $E_1 \approx$ or $< E_2$, the curvature radii in the x and y directions can be expressed as

$$\begin{aligned} 1/R_x &= \frac{6d_1[(E_{2y}E_{1x}\Delta\epsilon_{\alpha x} + \nu_{1y}\Delta\epsilon_{\alpha y}) - \nu_{2y}E_{2x}E_{1y}(\Delta\epsilon_{\alpha y} + \nu_{1x}\Delta\epsilon_{\alpha x})]}{d_2^2E_{2x}E_{2y}(1-\nu_{1x}\nu_{1y})}, \\ 1/R_y &= \frac{6d_1[(E_{2x}E_{1y}\Delta\epsilon_{\alpha y} + \nu_{1x}\Delta\epsilon_{\alpha x}) - \nu_{2x}E_{2y}E_{1x}(\Delta\epsilon_{\alpha x} + \nu_{1y}\Delta\epsilon_{\alpha y})]}{d_2^2E_{2x}E_{2y}(1-\nu_{1x}\nu_{1y})}, \end{aligned} \tag{11}$$

where

$$\Delta\epsilon_{\alpha x} = \int_{T_i}^{T_f} (\alpha_{2x} - \alpha_{1x})dT,$$

$$\Delta\epsilon_{\alpha y} = \int_{T_i}^{T_f} (\alpha_{2y} - \alpha_{1y})dT.$$

With the same assumption made above, by substituting Eq. (10) back into Eq. (4), the average film stress can be obtained:

$$\begin{aligned} \sigma_{1x} &= \frac{F_{1x}}{Wd_1} = \frac{d_2^2E_{2x}(R_y + \nu_{2y}R_x)}{6R_xR_y(1-\nu_{2x}\nu_{2y})d_1}, \\ \sigma_{1y} &= \frac{F_{1y}}{Wd_1} = \frac{d_2^2E_{2y}(R_x + \nu_{2x}R_y)}{6R_xR_y(1-\nu_{2x}\nu_{2y})d_1}. \end{aligned} \tag{12}$$

As shown, the curvature radii in the two directions orthogonal to each other must be determined separately so that stresses in the two different directions can be calculated. Usually, a minimum length of a given substrate is needed in order to measure precisely its curvature in one direction. Therefore, to perform experiments for these calculations, any elastically anisotropic substrate to be applied must be long and wide enough. Apparently, typical circular or D-shape wafers with appropriate diameter would be adequate.

It is noteworthy that the above expressions, derived according to the three balance equations, can also be separately obtained from an entirely different approach. That can be done by starting with the expression for the structure deflection of an elastically anisotropic plate obtained by Hearmon.[25] As to stress formulas, both methods give the same results, which can be used to ensure the correctness of this newly developed model.

For the elastically isotropic case, in which $E_{ix} = E_{iy}$, $R_x = R_y$, and $\nu_{ix} = \nu_{iy}$, the above expressions become

$$\sigma_{1x} = \sigma_{1y} = \sigma_1 = \frac{d_2^2E_2}{6R(1-\nu_2)d_1}.$$

This expression is commonly seen in models for isotropic bilayer structures.

D. Stress due to thermal mismatch

Stress arising in a thin film due to thermal mismatch can be described by Eq. (3). Since the stress variation in the thin film due to bending is relatively small and can be ignored, the relationship of the film stress with the thermal mismatch can be simplified as

$$\sigma_{1x} = \frac{E_1}{(1-\nu_1^2)}\left(\int_{T_i}^{T_f}(\alpha_{2x}-\alpha_1)dT + \nu_1\int_{T_i}^{T_f}(\alpha_{2y}-\alpha_1)dT\right), \quad (13a)$$

$$\sigma_{1y} = \frac{E_1}{(1-\nu_1^2)}\left(\int_{T_i}^{T_f}(\alpha_{2y}-\alpha_1)dT + \nu_1\int_{T_i}^{T_f}(\alpha_{2x}-\alpha_1)dT\right). \quad (13b)$$

Here, the properties of the thin film have been assumed isotropic so that the above expressions can be used to compare with those of Janda.[16] Apparently, the stress-thermal mismatchment relations we have obtained here are different from those of Janda.[16] Since the above expressions result directly from the three balance equations, they should undoubtedly be correct. On the contrary, Janda did not establish his stress-thermal mismatch relations on any theoretical basis or experimental support. By using his own formulas, which are incorrect, Janda has obtained very unreasonable Young's modulus and thermal expansion of the aluminum thin film deposited on an α-quartz substrate.

Again, for an elastically isotropical case, one has

$$\sigma_{1x} = \sigma_{1y} = \sigma_1 = \frac{E_1}{(1-\nu_1)}\int_{T_i}^{T_f}(\alpha_2-\alpha_1)dT. \quad (14)$$

If a thin film is deposited or grows on a Si circular wafer, which is the most common type of substrate utilized, the above simplified equation can be applied because the Si wafer is elastically isotropic in the (100) or (111) planes.

According to Eq. (13), if the structure is thermally cycled, the stress changes with respect to temperature at any given temperature in the thin film in the two different directions can be written as

$$\frac{d\sigma_{1x}}{dT} = \frac{E_1}{(1-\nu_1^2)}[(\alpha_{2x}-\alpha_1)+\nu_1(\alpha_{2y}-\alpha_1)], \quad (15a)$$

$$\frac{d\sigma_{1y}}{dT} = \frac{E_1}{(1-\nu_1^2)}[(\alpha_{2y}-\alpha_1)+\nu_1(\alpha_{2x}-\alpha_1)]. \quad (15b)$$

These results are, of course, different to those reported by Janda.[16] According to Janda's Eqs. (1) and (2), one will have different expressions, which are incorrect and have been used in Janda's calculations, as follows:

$$\frac{d\sigma_{1x}}{dT} = \frac{E_1}{(1-\nu_1)}(\alpha_{2x}-\alpha_1),$$

$$\frac{d\sigma_{1y}}{dT} = \frac{E_1}{(1-\nu_1)}(\alpha_{2y}-\alpha_1).$$

If these were correct, no further assumption would be needed in order to calculate the biaxial modulus and thermal-expansion coefficient of the thin film, since these are their only two unknown parameters, and there are two independent equations. However, as can be seen in Eq. (15), there are three unknown parameters for a given thin film. They are the thin film's Young's modulus, Poisson's ratio, and thermal-expansion coefficient. The Young's modulus and Poisson's ratio in the expression cannot be combined as a biaxial modulus, and therefore must be individually dertermined. There are, however, only two independent equations. It means that without making further assumptions, such an anisotropic substrate approach cannot be used to experimentally determine the mechanical constants and thermal-expansion coefficient of any given thin-film material. Apparently, this approach is not better than the approach of using two different isotropic substrates.

Nevertheless, this approach still has its own unique advantage. By knowing the thermal-expansion coefficient of the thin film, both the Young's modulus and Poisson's ratio can be individually determined. In the other approach, only the biaxial modulus can be obtained. Or, in this approach, if the Poisson's ratio of the thin film is known, both the thermal-expansion coefficient and Young's modulus can then be determined. In the next section, the mechanical constants and thermal-expansion coefficient of the aluminum thin film used by Janda will be given and discussed after being recalculated by using our model.

In Janda's study,[16] in order to verify his proposed model, thin aluminium films were deposited onto unheated circular substrates of α quartz (AT and BT cut) of 0.12 mm thickness and 15.5 mm diameter. The α-quartz substrate is elastically anisotropic and has Young's moduli of 7.831 and 9.066×10^{10} Pa, Poisson's ratios of 0.277 and 0.321, and thermal-expansion coefficients of 13.71 and 9.58×10^{-6}/°C, respectively, in the x and y directions. Since the α-quartz substrate exhibits significant elastic anisotropy and a circular substrate has been applied, the experimental data obtained by Janda should be good.

III. RESULTS AND DISCUSSION

Table I compares the Young's moduli, Poisson's ratios, and thermal-expansion coefficients of the aluminum thin film, calculated by using different models, with those of the bulk aluminum. When assuming that the thermal-expansion coefficient of the thin film is equal to that of the bulk, by using our model, the recalculated Young's modulus and Poisson's ratio are 4.2×10^{10} Pa and 0.41, respectively, for the film, whereas 6.9×10^{10} Pa and 0.35 are the values for the bulk. The recalculated biaxial modulus of the film is 7.2×10^{10} Pa, which is smaller than that of the bulk, but not too small. The biaxial modulus of the bulk aluminum is 10.6×10^{10} Pa. This result is not unusual since thin-film materials deposited on substrates are mostly in a strained state, and are likely to exhibit stress relaxation, especially when having defects. Consequently, the resulting relaxation mod-

TABLE I. Comparison of aluminum thin-film mehanical properties and the thermal-expansion coefficient calculated by using different models with those of bulk aluminum.

Material characteristics	Model used	Calculated		Results	
		$E/(1-\nu)(10^{10}$ Pa)	$E(10^{10}$ Pa)	ν	α(ppm/°C)
	Janda's model[a]	3.0	...	...	41
Thin film	Our model:				
	assumption 1	6.2	4.0	...	26
	assumption 2	7.2	4.2	0.41	...
Bulk	...	10.6	6.9	0.35	23.9

[a] See Ref. 16.

uli (or tensile moduli) are smaller when compared with those of the bulk. Actually, as also indicated in the literature,[10-11] thermally evaporated copper thin films and *e*-beam-evaporated copper thin films have lower tensile moduli as compared with that of the bulk.

The biaxial modulus calculated by using Janda's formulas, which are incorrect as mentioned earlier, is 3.0×10^{10} Pa. This value is too small to be true. However, by using our model, the mechanical properties of the aluminum thin film after recalculation have become much more reasonable. Furthermore, the recalculated Poisson's ratio, 0.41, is close to that of bulk, 0.35. All these results indicate that the assumption made above seems adequate.

When assuming that the Poisson's ratio of the thin film is equal to that of the bulk, the recalculated Young's modulus and thermal-expansion coefficient are 4.1×10^{10} Pa and 26.0×10^{-6}/°C for the thin film, and 6.9×10^{10} Pa and 23.9×10^{-6}/°C for the bulk. Again, the recalculated biaxial modulus of the film is smaller than that of the bulk, but not too small. The recalculated thermal-expansion coefficient of the thin film is very close to that of the bulk. These results indicate that the assumption made here is acceptable.

The thermal-expansion coefficient calculated by Janda is 41×10^{-6}/°C, which is nearly two times of that of the bulk. Such an unreasonably large discrepancy between the thermal-expansion coefficients of the thin film and the bulk can result from Janda's incorrect formulas. However, after recalculation by using our model and with the appropriate assumptions, the properties of the aluminum thin film have become much more acceptable.

IV. SUMMARY

In this paper, a newly developed model for analyzing stresses and curvatures in elastically anisotropic bilayer structures is presented. This model can be applied to bilayer structures composed of a single thin film that is deposited or grows on an elastically anisotropic substrate. The thin-film materials considered can be either elastically isotropic or anisotropic. According to the calculations shown here by using this model, it can be concluded that without making assumptions, the Young's modulus, Poisson's ratio, and thermal-expansion coefficient of any deposited thin film cannot be determined by simply using a single elastically anisotropic substrate. By using our model and with reasonable assumptions, the recalculated mechanical constants and thermal-expansion coefficient of the aluminum thin film, as presented by Janda, have become much more acceptable.

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